

Suppression of Quantum Scattering in Strongly Confined Systems

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Abstract

We demonstrate that scattering of particles strongly interacting in three dimensions (3D) can be suppressed at low energies in a quasi-one dimensional (1D) confinement. The underlying mechanism is the interference of the *s*- and *p*-wave scattering contributions with large *s*- and *p*-wave 3D scattering lengths being a necessary prerequisite. This low-dimensional quantum scattering effect might be useful in “interacting” quasi-1D ultracold atomic gases, guided atom interferometry and impurity scattering in strongly confined quantum wire-based electronic devices.

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In a scattering process the boundary conditions play a key role and can substantially affect the scattering outcome. In case of asymptotically free motion and for spherically symmetric potentials, it is natural to analyze the scattering processes using partial waves belonging to certain angular momenta. Consider then a scattering event in 3D between two distinguishable particles with relative momentum k . Adding contributions of higher partial waves with increasing orbital angular momentum l and phase shifts δ_l can only *increase* the total cross-section, which in 3D is given by

$$\sigma = \frac{4\pi}{k^2} \sum_l (2l + 1) \sin^2 \delta_l. \quad (1)$$

A pure s -wave ($l = 0$) approximation may not be accurate even at low energies for potentials that possess a significant spectral structure, e.g., impurity or dopant scattering in some bulk solid state systems [1, 2] or p -wave ($l = 1$) interactions in ultracold atomic physics [3, 4, 5, 6, 7, 8, 9, 10]. Such additional scattering terms for different partial waves could lead to increased heat dissipation along bulk conduction channels or to higher phase degradation in atom interferometry [11, 12, 13] due to atomic collisions.

The scattering process can change dramatically if it takes place in a partially confined geometry, such as quasi-1D systems. The latter situation is encountered in certain quantum wires [14, 15, 16, 17] for electronic transport or in wave guides for ultracold atoms [10, 18, 19, 20, 21]. Of particular interest is the single mode regime, where only the ground state (hereafter indicated by the index 0) with respect to the confining directions can be actually populated. Then, instead of σ , the quasi-1D total cross-section is the reflection coefficient R , which can be written in terms of the effective quasi-1D forward ($z \rightarrow +\infty$) scattering amplitude f_0^+ [18, 19, 20, 22],

$$R = 1 - |1 + f_0^+|^2, \quad f_0^+ = f_{0g} + f_{0u}, \quad (2)$$

where f_{0g} and f_{0u} are even and odd quasi-1D amplitudes containing even and odd partial l -waves, respectively. In a seminal work [18], in the s -wave approximation for which $f_{0u} \approx 0$, a resonance $R \approx 1$ has been predicted with $f_{0g} \approx -1$. The corresponding low energy transport is thus almost blocked and the longitudinal motion exhibits a near infinite effective quasi-1D scattering: the original confinement induced resonance (CIR) [18]. An account of the center of mass motion of colliding particles in the pure s -wave zero-range approximation is provided in [23]. On the other hand, higher partial wave contributions like the next p -wave

[6, 7, 8, 9, 10, 20, 22] in f_{0u} can also exhibit a resonance [20] with $f_{0u} \approx -1$. This is another diverging effective interaction, but in the odd sector [20].

The present work addresses the novel situation where a *simultaneous* resonance in the s - and p -wave scattering occurs such that $R \approx 0$. We show that the even and odd contributions to the scattering amplitude interfere and may provide effectively a quasi-1D gas of non-interacting atoms or a free flow of carriers in a quantum wire. Note, that this free flow occurs in spite of a strong interaction in 3D. We remark that for cold atoms dc electric field can supply us with hybridized Feshbach resonances providing a situation where both s - and p -wave scattering becomes simultaneously resonant [24]. The above-mentioned complementary or “dual” CIR due to both large s - and p -wave scattering is established by extracting the transmission $T = 1 - R = |1 + f_0^+|^2$ from the wave packet dynamical solution of the time-dependent Schrödinger equation for two particles with masses $m_1 \neq m_2$ and by highlighting the key concepts at play. The external transverse confinement is assumed to be parabolic $U_i(\rho_i) = \frac{1}{2}m_i\omega_i^2\rho_i^2$ where $\mathbf{r}_i = (\boldsymbol{\rho}_i, z_i)$, $i = 1, 2$, are the coordinates of the particles. Their interaction is the screened Coulomb potential ($V_0 < 0$)

$$V(r) = V_0 \frac{r_0}{r} e^{-r/r_0}, \quad (3)$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2|$ and r_0 is the screening length. Note that only for $\omega_1 = \omega_2$ the center of mass decouples and e.g. an impurity-like scattering can be described solely by the relative coordinates. If $\omega_1 \neq \omega_2$, a two-species gas of ultracold trapped atoms, e.g., ^{40}K , ^{85}Rb , ^{87}Rb and combinations thereof, can be described qualitatively, since only the low-energy asymptotic behaviour of the scattering process is required, which should depend mostly on properties such as the scattering lengths and the range of the potential V . Independent simulations with other potentials, e.g., C_6-C_{12} [19] or hyperbolic-cosine [20] are expected to provide the same behaviour and properties. Additionally Eq.(3) allows for a good control of the low energy scattering lengths by tuning its spectrum via V_0 . The computation of T is first performed for $\omega_1 = \omega_2$ and second for $\omega_1 \neq \omega_2$, including the coupling to the center of mass.

In the Schrödinger equation, the center of mass coordinates $\mathbf{R} = \frac{m_1}{M}\mathbf{r}_1 + \frac{m_2}{M}\mathbf{r}_2$, with $M = m_1 + m_2$, are employed in the cylindrical representation (ρ_R, ϕ_R, Z) while for the relative coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, depending on the representation both cylindrical (ρ, ϕ, z) and spherical coordinates (r, θ, ϕ) are needed. By symmetry, the motion with respect to the

degree of freedom Z can be decoupled from the problem and will be omitted. In addition, due to the conservation of the z -component of the total angular momentum, namely, $L_{1z} + L_{2z} = -i(\partial_{\phi_1} + \partial_{\phi_2}) = -i(\partial_\phi + \partial_{\phi_R})$, ϕ_i being the azimuthal angle of \mathbf{r}_i ($\hbar = 1$), the number of independent variables can be further reduced in a frame co-rotating with the center of mass around the symmetry z -axis. This is accomplished by the unitary transformation [25]

$$\hat{\mathcal{U}} = e^{i\phi_R L_z}, \quad (4)$$

where $L_z = -i\partial_\phi$. Expressing the total Hamiltonian in terms of $\rho_R, \phi_R, r, \rho, \theta$ and ϕ , the net effect of this transformation is to shift ∂_{ϕ_R} to $\partial_{\phi_R} - \partial_\phi$ in the kinetic operator for the center of mass and ϕ to $\phi + \phi_R$ in the potential operator that couples ρ to ρ_R . The rotated Hamiltonian without V becomes then

$$H_0 = H_M + H_\mu + W. \quad (5)$$

Here $H_M = -(\partial_{\rho_R}^2 + 1/4\rho_R^2)/2M - (\partial_{\phi_R} - \partial_\phi)^2/2M\rho_R^2$, $W = \frac{1}{2}M\omega_M^2\rho_R^2 + \frac{1}{2}\mu\omega_\mu^2\rho^2 + \mu(\omega_1^2 - \omega_2^2)\rho\rho_R \cos\phi$ and $H_\mu = -\partial_r^2/2\mu + L^2/2\mu r^2$, where L^2 is the square of the orbital angular momentum of the relative coordinates with eigenvalues $l(l+1)$, $\mu = m_1 m_2 / M$ is the reduced mass, $\omega_\mu^2 = (m_2/M)\omega_1^2 + (m_1/M)\omega_2^2$ and $\omega_M^2 = (m_1/M)\omega_1^2 + (m_2/M)\omega_2^2$ characterize the confinement oscillator frequencies for the relative and center of mass coordinates, respectively, whereas V is invariant with respect to the transformation $\hat{\mathcal{U}}$. The derivative ∂_ϕ in the second term of H_M is a Coriolis coupling term, which is characteristic for the rotating frame of reference and appears as an additional kinetic energy operator.

The initial wave packet at $t = 0$ possesses a Gaussian shape of width a_z and momentum $k_0 \equiv \sqrt{2\mu\varepsilon} > 0$ for the unconfined z -motion

$$\Psi(0) = Nr\sqrt{\rho_R} [\hat{\mathcal{U}}\Phi] e^{-(z-z_0)^2/2a_z^2} e^{izk_0}, \quad (6)$$

N is the overall normalization constant defined as $\langle \Psi(0) | \Psi(0) \rangle = \int_0^\infty dr \int_0^\infty d\rho_R \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \Psi^*(0)\Psi(0) = 1$ and the particles are separated by $z_0 < 0$ while their confined motions ρ_i are in the respective harmonic oscillator ground state $\Phi = \Phi(\rho_1, \rho_2) = e^{-(\rho_1^2/a_1^2 + \rho_2^2/a_2^2)/2}$ with $a_i = (1/m_i\omega_i)^{1/2}$. By expressing ρ_i in terms of the variables ρ_R, ϕ_R, ρ and ϕ , the action of $\hat{\mathcal{U}}$ is to simply shift ϕ to $\phi + \phi_R$ in the exponent of Φ , as can be seen by using the basis of eigenstates of L_z . As a result, the ϕ_R variable drops from the initial state $\Psi(0)$ and the Schrödinger equation $i\dot{\Psi}(t) = [H_0 + V]\Psi(t)$

reduces to the subspace of the four variables (ρ_R, \mathbf{r}) . The z -component of the total angular momentum is in the co-rotating frame given by $L_Z = -i\partial_{\phi_R}$. According to our initial wave packet in Eq.(6) we assume now a vanishing total angular momentum $L_Z\Psi = 0$ and therefore omit the corresponding derivative terms in H_M .

The extraction of T from $\Psi(t)$ follows from the asymptotics at large times t , when $\Psi(0)$ has been split by V into a backward and a forward scattered part outside the range of V ideally for $z \rightarrow \mp\infty$, respectively. It can be obtained from the forward scattered part by integrating the asymptotic density $|\Psi(t)|^2$ over the half-space $z \geq r_0$ or from the projection $|\langle \Psi_0(t) | \Psi(t) \rangle|^2 \xrightarrow[t \rightarrow \infty]{} |1 + f_0^+|^2$ onto the *unscattered* large t evolution of $\Psi(0)$ under H_0 alone. In the limit $a_z \rightarrow \infty$ our wave packet scattering corresponds asymptotically ($t \rightarrow \infty$) to the monoenergetic stationary scattering situation thereby providing the energy or momentum resolved scattering parameter $T = T(k)$.

The present computational scheme to solve for $\Psi(t)$ is a four dimensional extension of a three dimensional method originally developed to treat, among others, bound-bound and bound-continuum transitions for atomic systems in external fields [26, 27, 28]. In this scheme, an angular basis $f_j(\theta, \phi)$ is constructed on the grid (θ_j, ϕ_j) using the exponentials $e^{im\phi}$ and the Legendre function $P_l^m(\theta)$, such that the only non-diagonal terms are the angular parts of the kinetic energy operators, namely, $L^2/2\mu r^2$ and $-\partial_\phi^2/2M\rho_R^2$. These, in turn, can be diagonalized efficiently if one employs additionally a simple unitary transformation between the two basis f_j and $e^{im\phi}$, $P_l^m(\theta)$ [26, 28]. Our approach is reminiscent of a two dimensional discrete variable representation (DVR) [29] and the values of the wave function $\Psi(t)$ are given on an angular grid (θ_j, ϕ_j) whose total number of grid points equals the number of basis functions f_j . The solution is then propagated in time using a component-by-component split-operator method [26, 28] according to $\Psi(t + \Delta t) \approx e^{-\frac{i}{2}W\Delta t} e^{-i(H_\mu + V)\Delta t} e^{-iH_M\Delta t} e^{-\frac{i}{2}W\Delta t} \Psi(t)$.

To be specific the parameters are chosen as follows. $r_0 = 1$ defines the length scale, $m_1/m_2 = 40/87$ is the mass ratio (e.g., ^{40}K and ^{87}Rb) and the reduced mass is taken as the unit mass $\mu = 1$. We define $\omega = (\omega_1 + \omega_2)/2$ and the confinement length $a_\perp \equiv \sqrt{1/\mu\omega}$. For the case of a decoupled center of mass motion, $\omega_1 = \omega_2 = \omega$, whereas for the coupled case, $\omega_1 = 1.35\omega_2$. The low longitudinal energy $\varepsilon = 0.002$ guarantees the single mode regime $\omega < E = \omega + \varepsilon < 3\omega$ for the region of $0.002 \leq \omega \leq 0.02$ we consider.

For $-V_0 < 9$ (in units of $\hbar^2/\mu r_0^2$), there exists no bound-state of $V(r) + l(l+1)/2\mu r^2$ for $l \geq 2$. Thus only the s - and p -wave 3D scattering lengths a_s and a_p can be large. These

are computed in the limit $k \rightarrow 0$ by $k \cot \delta_0(k) = -1/a_s$ and $k^3 \cot \delta_1(k) = -1/V_p$, with $V_p \equiv a_p^3$.

First let us consider the confined scattering process for the case of a decoupled center of mass motion $\omega_1 = \omega_2 = \omega$. The results for T are shown in Fig. 1 together with the behaviour of the 3D scattering lengths a_s and a_p . These are tuned by changing V_0 in two regions where correspondingly only a_s ($-V_0 \sim 1$) or both a_s and a_p ($-V_0 \sim 7.5 - 9.5$) are large, i.e., on the order of a_\perp . In the first region we see the well-known s -wave CIR which leads to a minimum $T \approx 0$ when the ratio a_\perp/a_s approaches $a_\perp/a_s \approx 1.46$ in agreement with [18, 19]. In the second region, however, remarkable peaks $T \approx 1$ in the transmission are observed being most pronounced for small momenta k_0 (small a_\perp). Considering in this case pure s -wave scattering would yield $T \approx 0$ [18] in contrast to the behaviour $T \approx 1$ shown in Fig. 1. Clearly this is due to the fact that both a_s and a_p become large and contribute equally to the scattering process. We therefore encounter the peculiar situation of an almost complete transmission, i.e. free flow, in spite of the strong interaction between the scattering partners in free space.

This effect of the suppression of the quantum scattering ($T \approx 1$) for $-V_0 \sim 8 - 9$ is encountered equally in the case of a coupling with the center of mass $\omega_1 \neq \omega_2$ (see Fig. 2). The position $a_\perp/a_s \approx 1.45$ of the total transmission for $\omega_1 = \omega_2 = 0.02$ is only slightly shifted to $a_\perp/a_s \approx 1.25$ under the action of the coupling with the center of mass for $\omega_1 = 1.35\omega_2$ and the maximum of T is slightly decreased. Note that in strong contrast to T , the 3D cross section σ , e.g. for $V_0 = -8.45$ and $E \sim \omega_1 = \omega_2 = 0.02$, can increase almost four-fold if the p -wave contribution is added.

The observed dramatic change of T due to the combined action of s - and p -wave scattering is qualitatively confirmed in simpler though solvable models, at least in the absence of the coupling to the center of mass. Indeed, for $\omega_1 = \omega_2$ and $kr_0 = \sqrt{2\mu E}r_0 \ll 1$ (i.e., low total energy), the condition equivalent to $f_{0u} \approx -1$ can be obtained separately from the antisymmetric part of the wave function as a divergence of a quasi-1D effective interaction strength for $a_\perp/a_p = -1.36$ [20, 30]. Together with $a_\perp = 1.46a_s$ [18], one finds again the requirement of both large a_s and a_p . Another more direct determination of both $f_{0g,u}$ using the approximation developed in [22] predicts $a_\perp = 2a_s = -2a_p$, namely, $f_{0g} = -(1 + i \cot \delta_g)^{-1}$ and $f_{0u} = -(1 + i \cot \delta_u)^{-1}$, where $\cot \delta_g = -[a_\perp/a_s - (C^2 - a_\perp^2 k_0^2)^{1/2}]a_\perp k_0/2$ while $\cot \delta_u = -[a_\perp^3/V_p + (C^2 - a_\perp^2 k_0^2)^{3/2}]/(6a_\perp k_0)$ is a straightforward improvement to Eq.(30b)

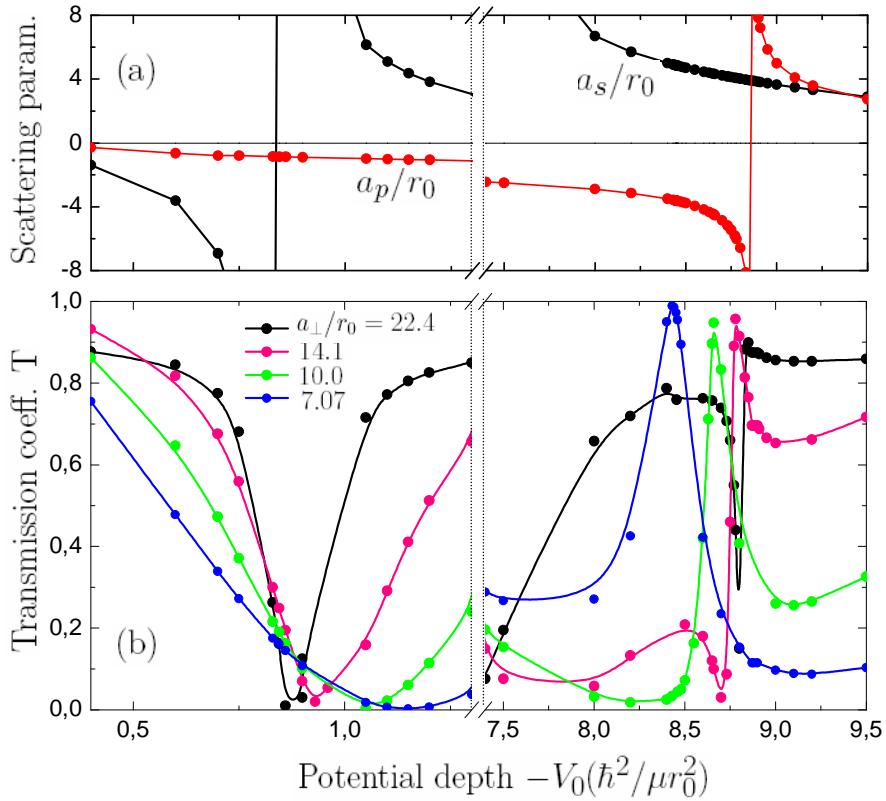


FIG. 1: (color online) (a) The 3D scattering lengths a_s (black) and a_p (red) and (b) the quasi-1D transmission coefficients T for a few values of a_\perp and fixed $\varepsilon = 0.002$ ($k_0 = 0.0632$). Discussion see text.

of Ref. [22] and $C = 2$. Using then $a_s(V_0)$ and $a_p(V_0)$ of a square-well of depth V_0 and radius r_0 in the scattering amplitudes $f_{0g,u}$ we obtain T from Eq.(2) which is shown in Fig. 3. The resulting behavior is qualitatively similar to Fig. 1, confirming the role of both large a_s and a_p , on the order of a_\perp .

For an experiment, the main condition for $T \approx 1$ is $f_{0g,u} \approx -1$. If the partial waves $l \geq 2$ are negligible and $k_0 r_0 \ll kr_0 \ll 1$, this results in the fact that a_s and $-a_p$ are of the order of a_\perp . More precise values of these ratios [18, 20] may depend on details of the confining potential, coupling to the CM, k_0 , and should be computed for a given experimental setup. Current laser traps for e.g. ^{40}K can well reach the ranges $a_s \sim a_\perp < 60\text{nm}$ [31] or $-a_p \sim a_\perp < 60\text{nm}$ [10], using, however, *separate* 3D Feshbach resonances in the s - and p -waves [6]. In a recent paper [24] a mechanism for the *simultaneous* creation of s - and p -wave Feshbach resonances is established: Applying laboratory dc-electric fields introduces the herefore necessary mixing of s - and p - waves. Thus, a reduction of quasi-

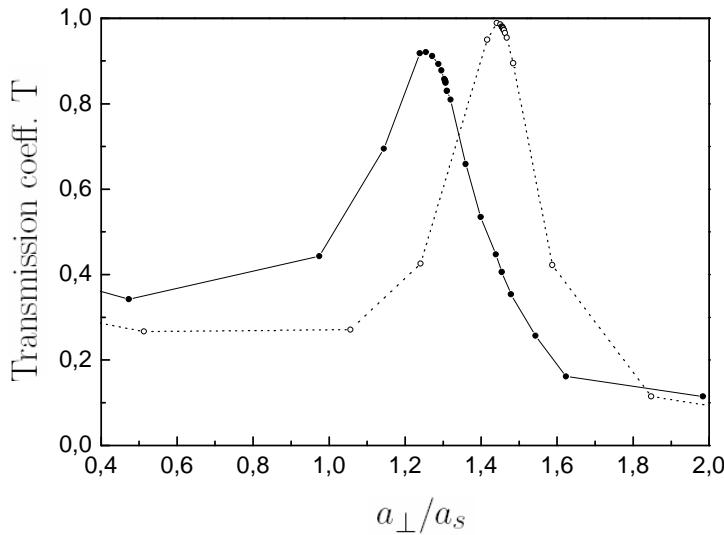


FIG. 2: The influence of the center of mass coupling on the transmission T for $\omega_2 = 0.02$ and $\varepsilon = 0.002$. Here $\omega_1 = 1.35\omega_2$, $a_{\perp}/r_0 = 6.52$ (solid curve) and $\omega_1 = \omega_2$, $a_{\perp}/r_0 = 7.07$ (dotted curve).

1D scattering relative to 3D, as revealed e.g. in trap losses, should be observable with tighter traps by further exploring Feshbach resonances. Another example is the potential $V = -(Z_i e^2 / \kappa r) e^{-r/r_0}$ of an ionized impurity of valence Z_i in a semiconductor quantum wire with dielectric constant κ . Restoring the length unit r_0 , the relation to V_0 (in units of $\hbar^2 / \mu r_0^2$) is thus $r_0 = -\kappa \hbar^2 V_0 / Z_i \mu e^2$. For $V_0 = -8.45$, the required screening length r_0 can range from 5.4 nm (heavy holes in Si and $Z_i = 2$) up to 86.8 nm (electrons in GaAs and $Z_i = 1$). Geometrically, this range and $a_{\perp} \gg r_0$ are well within current scaling technologies [17].

In conclusion, due to quantum interference of different partial wave amplitudes, the scattering in a quasi-1D geometry can be strongly suppressed, although the interaction or scattering in 3D is strong.

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[1] E. Conwell and V. Weisskopf, Phys. Rev. **77**, 388 (1950).

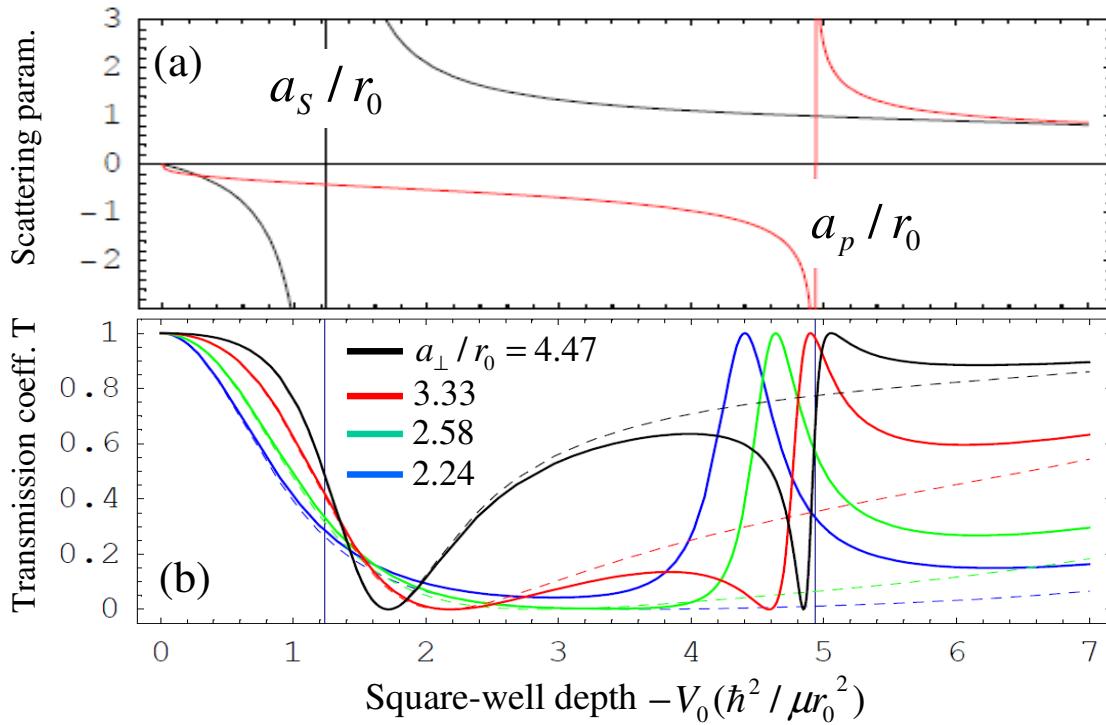


FIG. 3: (color online) Scattering lengths and transmission for the square-well potential (depth V_0 and radius r_0) for $\omega_1 = \omega_2$ and $\varepsilon = 0.04$. (a) $a_s = a_s(V_0)$ (black) and $a_p = a_p(V_0)$ (red). (b) $T = T(V_0)$ for several values of a_\perp [see Fig.(1b)]. For comparison, f_{0u} is omitted in the dashed curves and only the s-wave CIR behaviour $T \approx 0$ due to large a_s appears.

- [2] B.K. Ridley, *Quantum Processes in Semiconductors* (Oxford University Press, USA, 4th Ed., 2000).
- [3] L. Santos *et al.*, Phys. Rev. Lett. **85**, 1791 (2000).
- [4] L. Santos, G.V. Shlyapnikov and M. Lewenstein, Phys. Rev. Lett. **90**, 250403 (2003).
- [5] J. Stuhler *et al.*, Phys. Rev. Lett. **95**, 150406 (2005).
- [6] C. Ticknor *et al.*, Phys. Rev. A **69**, 042712 (2004).
- [7] R. Stock *et al.*, Phys. Rev. Lett. **94**, 023202 (2005).
- [8] L. Pricoupenko, e-print cond-mat/0508120 (2005).
- [9] Z. Idziaszek and T. Calarco, Phys. Rev. Lett. **96**, 013201 (2006).
- [10] K. Günter *et al.*, Phys. Rev. Lett. **95**, 230401 (2005).
- [11] M.D. Girardeau, K.K. Das and E.M. Wright, Phys. Rev. A **66**, 023604 (2002).
- [12] M. Jääskeläinen, W. Zhang and P. Meystre, Phys. Rev. A **70**, 063612 (2004).
- [13] T. Schumm *et al.*, Nature Phys. **01**, 57 (2005).

- [14] G.W. Bryant, Phys. Rev. B **29**, 6632 (1984).
- [15] C.S. Chu and R. Sorbello, Phys. Rev. B **40**, 5941 (1989).
- [16] D.S. Chuu and C.M. Hsiao and W.N. Mei, Phys. Rev. B **46**, 3898 (1992).
- [17] Y. Cui *et al.*, Nano Lett. **3**, 149 (2003).
- [18] M. Olshanii, Phys. Rev. Lett. **81**, 938 (1998).
- [19] T. Bergeman, M.G. Moore and M. Olshanii, Phys. Rev. Lett. **91**, 163201 (2003).
- [20] B.E. Granger and D. Blume, Phys. Rev. Lett. **92**, 133202 (2004).
- [21] R. Folman *et al.* Adv. At. Mol. Opt. Phys. **48**, 263 (2002).
- [22] J.I. Kim, J. Schmiedmayer and P. Schmelcher, Phys. Rev. A **72**, 042711 (2005).
- [23] V. Peano *et al.*, New J. Phys. **7**, 192 (2005).
- [24] R.V. Krems, Phys. Rev. Lett. **96**, 123202 (2006).
- [25] H. Bock, I. Lesanovsky and P. Schmelcher, J. Phys. B: At. Mol. Opt. Phys. **38**, 893 (2005).
- [26] V.S. Melezhik, Phys. Lett. A **230**, 203 (1997); in *Atoms and Molecules in Strong External Fields*, p. 89, editors P. Schmelcher and W. Schweizer (Plenum, New York, 1998).
- [27] V.S. Melezhik and P. Schmelcher, Phys. Rev. A **59**, 4264 (1999); V.S. Melezhik and P. Schmelcher, Phys. Rev. Lett. **84**, 1870 (2000).
- [28] V.S. Melezhik and C.-Y. Hu, Phys. Rev. Lett. **90**, 083202 (2003); V.S. Melezhik, J.S. Cohen and C.-Y. Hu, Phys. Rev. A **69**, 032709 (2004).
- [29] J.C. Light and T. Carrington, Jr., Adv. Chem. Phys. **114**, 263 (2000).
- [30] M.D. Girardeau and E.M. Wright, Phys. Rev. Lett. **95**, 010406 (2005).
- [31] H. Moritz *et al.*, Phys. Rev. Lett. **94**, 210401 (2005).